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News From Argonne's Transportation Technology R&D Center

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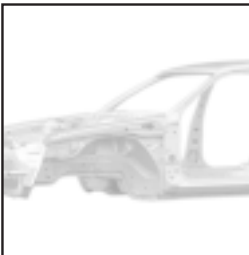


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■ VIEWPOINT

“X-Ray Vision”: Taking a Hard Look at Fuel Sprays and Combustion

Argonne researchers are collaborating on a close-up study of diesel spray patterns and soot formation using the Advanced Photon Source here at the Laboratory. The APS makes it possible for scientists to examine these phenomena closer than ever before. The knowledge gained could lead to better-performing, lower-emission injectors for modern automotive engines, as well as more efficient operation. *Page 2*



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■ RESEARCH REVIEW

Model Helps Focus Fuel Cell Vehicle Research

With the volatility of gas prices and ever more stringent emissions regulations, the automotive industry is being pressured to design clean, efficient, affordable vehicles. GCtool, a computer software package developed at Argonne, lets automotive designers try out different system configurations without the expense and delays of building numerous prototypes. *Page 4*

Argonne Predicts Benefits of Aluminum-Intensive Vehicles

Aluminum is energy-intensive to produce from scratch, but when it is recycled and reused in automotive applications, aluminum may yield some very attractive performance and environmental advantages over conventional steel. Using life-cycle analysis, Argonne determined that aluminum-intensive vehicles offer consumers better fuel economy and handling because of reduced weight, as well as a rust-proof body. *Page 5*



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Rail Lubricant Technology Goes High Tech

Argonne researchers are working with the rail industry on finding ways to make railroad technology safer and more cost-effective. We are assessing the environmental and tribological performance of a computerized lubrication system that applies lubricant to the tops of both rails after the last axle of the last locomotive at the front of the train passes by. The technology holds significant promise for reducing the cost and environmental effects of rail lubricants. *Page 6*

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“X-Ray Vision”: Taking a Hard Look at Fuel Sprays and Combustion

As a child, you might have owned a see-through model engine, made mostly out of transparent plastic, that let you see what was going on inside it: with the help of a tiny electric motor, fan blades twirled, pistons moved up and down, and the crankshaft really turned! The plastic model had no fuel system or working spark plugs, so you couldn’t actually watch combustion at work. Even today, engine researchers cannot directly observe all the details of critical combustion processes in a working engine. Thanks to groundbreaking research by Argonne scientists and engineers, however, the day of the “transparent” internal combustion engine is about to dawn at last. The secret? “X-ray vision!”

Teams of Argonne researchers are using high-brilliance x-rays from the Advanced Photon Source (APS) — a unique user facility dedicated to producing synchrotron x-rays for research — to shine a piercing new light on the fluid dynamics and chemistry of fuel spray behavior and combustion processes.

Seeing inside fuel sprays... a shocking discovery

A team of Argonne researchers is using APS x-rays to obtain never-before-possible quantitative data on the structure and behavior of cold gasoline and diesel sprays. Continuing and expanding on experiments reported previously [*TransForum*, Volume 2, No. 2, p. 5], Roy Cuenca, Yong Yue, Jin Wang, and Chris Powell are using x-ray adsorption techniques to fill a critical gap in our knowledge of spray behavior and dynamics.

The gasoline spray from an injector nozzle takes the form of a hollow cone — a thin sheet of particles on the outside, surrounding an empty-air interior. Using their experimental apparatus, Cuenca and his colleagues can obtain the instantaneous local mass of fuel in any given volume element. According to Wang, “with such information, the time resolution of APS x-rays lets us measure the thickness of the gasoline spray’s walls quantitatively; no one could do this before x-ray sources like the APS became available.” The measurements make it possible to say exactly how well the injector is atomizing the fuel, which may

provide useful insights into tip erosion, a common problem with fuel-injected engines.

Argonne’s diesel spray research is also yielding some new information. Until now, it was customary to regard the dense core of the diesel spray as a liquid, but the Argonne researchers — penetrating the region within the first five millimeters of the spray nozzle, where optical laser techniques are useless — have shown that the core is no more than about 50% liquid; the rest is trapped fuel/air vapor. This is an important finding about diesel combustion, a process limited mainly by the extent of fuel-oxygen mixing.

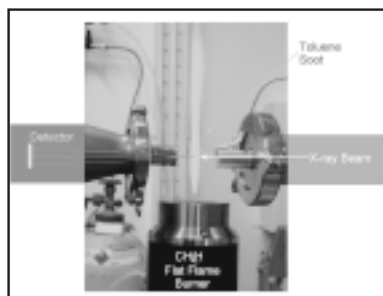
The team’s experiments also provided a surprise of major significance. Increased pressures are being used in modern injection systems to meet emissions regulations; at the higher pressures, internal cavitation can take place, disrupting the flow. In their spray experiment, the Argonne researchers were the first to detect evidence of a shock wave being formed. They showed their data to engineers at Robert Bosch in Germany, an industrial partner and leading developer of common-rail systems; the Bosch people were then able to obtain photographic proof of the shock wave’s existence. “In the injection cycle, the spray’s trailing edge moves faster than the leading edge, catching up with it and generating shock waves,” says Cuenca. “That’s why it happens. The question is, does the same thing happen under actual engine operating conditions? If so, can you prevent it... or even find a way to take advantage of it?”

With data from the spray experiments, it is no longer necessary to guess at conditions close to the injector nozzle. Engine manufacturers and designers of combustion devices will benefit from Argonne’s fuel-spray research. The knowledge gained could lead to higher-performance, lower-emission injectors for modern automotive engines, as well as more efficient operation.

Getting the dirt on soot

In a related effort, Argonne researchers are looking — more closely than anyone has before — at the formation of soot particles during combustion. When you look at a flame, the part that’s burning reddish-orange is produced by incandescent (“red-hot”) soot particles; the bluish central part of the flame is actually much hotter and contains no soot. By scattering x-rays off soot particles as they form inside a steady flame, Argonne chemists Jan Hessler, Randall Winans, and Al Wagner have determined soot particle distributions at sizes on the order of a nanometer (nm) — ten times smaller than can be achieved by optical laser techniques.

The scientists don’t actually measure individual soot particles, much less get visual images of them. They measure the intensity of the x-rays as a function of scattering angle, and by analyzing these data they can characterize the distributions of soot par-



By scattering x-rays off soot particles forming inside a flame, Argonne researchers identified particle distributions at sizes as small as one nanometer — ten times smaller than can be achieved by optical methods.



ticles in the line of the x-ray beam. The burner that produces the flame in their experiments can be moved vertically through the beam, changing the line of sight to sample the whole flame.

Mechanisms for soot growth are varied, but until now there's been little experimental evidence available for the early stages of growth. Distributions measured in laser experiments for particles in the 15-20 nm range can be calibrated with the Argonne researchers' x-ray data, filling in a vital information gap. The chemists' work opens up a region of soot growth that was previously inaccessible. "We're the first to obtain any data on soot formation at sizes of 1-2 nm and times on the order of a millisecond," says Hessler.

The nanometer-scale particles represent the earliest stage of soot formation ever seen. Models of soot formation are most sensitive to how events proceed in the earliest stages, so the researchers' experimental data provide critical information needed to validate such models. According to Wagner, "If we had a model, it would predict the distributions, which could then be compared with what we see experimentally."

As industry refiners use heavier oils (containing more soot-producing ingredients) in the fuel production process, particulate matter is likely to become more of a problem. Also, while the popular perception of air pollution is still focused on black puffs of smoke from trucks and buses, health experts are beginning to see the ultrafine, nanoscale particulates as a more serious concern. How can research on soot formation help? According to Winans, "Our research is applicable to a broad spectrum of environmental problems. Thus far, the approach to controlling emissions has been rather 'Edisonian,' but if we understand the mechanisms governing soot formation at its earliest stages, then we could control emissions much more effectively."

Taking the next step, and the next

Although the fuel-spray research has involved only cold sprays (and thus, no soot formation), it has the potential to complement the combustion studies. Winans's team found soot particles smaller than any ever observed before, and that knowledge could be helpful in future spray experiments. The researchers are planning a joint effort to study both cold and ignited sprays. The project requires that a new instrument be designed for studying spray breakup with and without ignition, in hopes of correlating soot formation and spray breakup.

"Soot formation presents both chemical and fluid mechanical problems," says Wagner. "Diesel spray breakup is also fluid mechanical. They measure density variations in the spray — we plan to coordinate our soot formation work with the spray research under more realistic combustion conditions."

The fuel-spray and soot-formation experiments at the APS have

demonstrated the advantages of x-ray research at ambient temperature and pressure — the next step is to study these phenomena under more realistic engine operating conditions (temperatures of many hundreds of degrees Celsius, pressures of several atmospheres), which will require making pressurized chambers x-ray-accessible ("windows" transparent to x-rays). The new, integrated instrument being designed for both cold and ignited spray studies won't be a real engine, because it will include no piston. But a temperature-pressure environment could be achieved that approaches actual diesel engine conditions. Such a device could serve as the forerunner for an eventual x-ray engine research center based at the APS. X-rays would pass through a test engine running under realistic conditions to study oxidation, formation of NO_x and particulates, etc.

"Engine researchers have been using 'paper engines' — computer simulations based on computational fluid dynamics — but the models aren't accurate enough," says Cuenca. "We've tried the 'optical engine' approach, using quartz-glass windows for laser access, but it cannot function at realistic engine temperatures or develop adequate power. But if some day we can build an 'x-ray engine,' then we can find out exactly what happens inside it under real-world conditions. That will mean a new paradigm in engine diagnostics."

Argonne's fuel-spray research is supported by the U.S. Department of Energy's Office of Transportation Technologies, with additional funding from the researchers' industrial partners, Robert Bosch, Outboard Marine, and Delphi Systems. The research on soot formation is supported by the Department's Office of Basic Energy Sciences (Office of Science, Division of Chemical Sciences).



Jin Wang (APS-UPD), Randy Winans (CHM), Roy Cuenca (ESD), and Chris Powell (APS-UPD) examine an experimental setup that will be used to study diesel spray breakup and soot formation under more realistic operating conditions at the APS.



Model Helps Focus Fuel Cell Vehicle Research

It's midnight in Michigan, and somewhere outside Detroit an automotive engineer is staring at the ceiling, wondering how she's going to squeeze 1% more efficiency out of the fuel cell reformer she's been working on. Never mind 5% more from the next component on her list.

When it comes to designing fuel cell and other next-generation vehicles, the pressure is on. With the volatility of gas prices and ever more stringent emissions regulations, the automotive industry is being squeezed as never before to design and bring to market highly efficient, environmentally friendly, affordable cars and trucks. Playing an essential role in this effort is computer software that lets designers "try out" different system configurations, without the expense and delays of actually building numerous prototypes.

An example of this software is the General Computational toolkit (GCtool), a versatile simulation software package that was developed by Argonne for designing, analyzing, and comparing different power-plant configurations. This flexible software uses a modular approach to integrate many of the detailed thermodynamic and component models developed during decades of fuel cell and power system research at Argonne and elsewhere.

GCtool is easy to use. "An entire fuel cell system — everything necessary to go from fuel to electricity — is specified as a sequence of lines of simple code," says Romesh Kumar, who leads Argonne's fuel cell modeling efforts. From this input, the software generates a system schematic, and users can switch between the input window and the diagram until they are satisfied with the flows. According to Kumar, "You enter lines in the input window and then you look at the diagram and say, 'Oh, wait a minute — this isn't going where I wanted,' and you go back and change it." All the input, including lines specifying the fuel, feed rates, and component performance, can fit on one page for a relatively simple system. The user can modify all the system inputs — down to the density and thickness of a heat exchanger wall.

Sensitivity analyses, one of the things the software is often used for, can save automotive engineers a tremendous amount of time. Kumar explains: "We might see that a small difference in the fuel cell performance yields a big difference in the vehicle efficiency, which means the whole system is very sensitive to that. Whereas if we change the airflow by a factor of two, the efficiency may not change much — then we can say the system isn't much affected by airflow, and we can focus our efforts elsewhere."

By questioning all of their assumptions, Argonne's systems analysis team found a surprise hiding in the compressor/expander systems used to manage water and operating pressure in fuel cell

systems — namely, that the efficiency of these systems is much more important to overall efficiency than expected.

The research for GCtool is supported by funding from the U.S. Department of Energy's Office of Transportation Technologies. As automotive fuel cell technology gets closer and closer to what promises to be a huge market, companies are naturally reluctant to reveal their research. The kind of analysis done at Argonne, because it can be made public, provides an important forum for discussion that can keep developers from working in isolation and spending energy, time, and money that could be devoted to more critical problems.

A variety of arrangements is available for licensing the technology. At present, about a dozen organizations outside of Argonne are using GCtool for systems analysis and evaluation. Some of these users are private-sector fuel cell companies and universities that assist DOE in the development of new fuel processing and fuel cell system technologies for automotive applications.

GCtool Features

The GCtool environment is highly user-friendly. System configurations are set up with lines of C-like code; model parameters are easily changed; and pop-up windows are used to display plots. Other important features of the model include the following:

- Offers four different types of fuel cells — proton exchange membrane (PEM), molten carbonate, phosphoric acid, and solid oxide cells.
- Provides detailed chemical and thermodynamic modeling of processes within the fuel cell stack.
- Is faster than most other systems.
- Includes complete energy and mass balance.
- Addresses blended fuels — it can represent the many hydrocarbons in gasoline and diesel fuels.

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Argonne Predicts Benefits of Aluminum-Intensive Vehicles

At the Paris Exposition of 1855, as part of the rich and varied displays of France's evolving industrialized culture, visitors were introduced to a light, shiny "precious metal" that would revolutionize modern living: aluminum.

Today, aluminum is no less precious than it was in 1855. From airplanes to pop cans, aluminum is an integral part of our daily lives. Aluminum is energy-intensive to produce from scratch, but Argonne researchers have recently found that — when it is recycled and reused in automotive applications — aluminum may yield some very attractive performance and environmental advantages over conventional steel.

Using life-cycle analysis, or LCA, Argonne's Frank Stodolsky and Linda Gaines have shown that aluminum-intensive vehicles, or AIVs, offer consumers key benefits: better fuel economy and handling because of reduced weight, plus a body that will not rust. "At a larger scale," explains Gaines, "our nation's economy would benefit by increasing the number of AIVs on the road because we would cut our consumption of petroleum; by reducing petroleum consumption, we would see lower emissions and cleaner air."

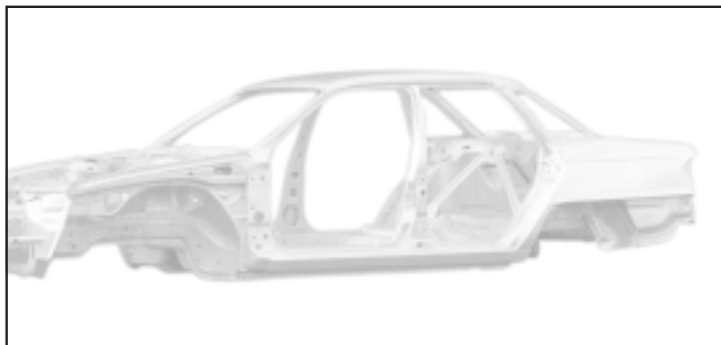
Assuming widespread commercialization of AIVs, Argonne's LCA projects that the United States should see petroleum energy savings of over 2% as soon as 2005 and 4.6% by 2030. Says Gaines, "Our study assumed constant engine performance, but engine technology keeps advancing and fuel economy keeps improving, particularly as vehicles become lighter." These improvements will further bolster the projected benefits of aluminum-intensive cars, particularly improvements in fuel economy.

The benefits do not end at improved fuel economy. Inch for inch, AIVs are between 20 and 30% lighter than conventional

steel vehicles, and they are equally safe. Explains Stodolsky, "An AIV will be just as safe as a steel car because it can be engineered with ample crush zones." Other benefits most obvious to consumers — as demonstrated by Argonne's on-site AIV Mercury Sable, which has accumulated 60,000 miles — include a durable body and improved fuel efficiency, compared with the conventional Sable.

Argonne researchers began their LCA by using a vehicle choice model to project market shares for various lightweight-vehicle options. The clear winner was the AIV. Explains Stodolsky, "Our study showed that the carbon fiber composite, another leading candidate lightweight material, was too costly for full fleet use, even assuming heroic reductions are possible in material production and manufacturing costs." Then, Argonne considered such key energy variables as vehicle fuel consumption, material production energy, and recycling energy. "In short," says Stodolsky, "we concluded that there is a net energy savings with the use of AIVs."

In the near term, however, using unrecycled aluminum is expensive, and at present, its large-scale use is limited to expensive specialty, luxury, or high-performance vehicles, not the types of cars most people drive every day. "All-aluminum-bodied cars are still rarities on today's roads and highways," notes Stodolsky. Over the long term, though, recycling wrought aluminum back to wrought aluminum saves even more energy than recycling other widely used vehicle materials. Ongoing advances in aluminum manufacturing and assembly technologies almost ensure that the cost of AIVs will drop to a point at which consumers have more vehicle choices than they do now.



Argonne is working with the automotive industry to evaluate the costs and benefits of aluminum-intensive vehicles.

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Rail Lubricant Technology Goes High Tech

"I ... have invented a new and useful improvement on locomotive-engines used on railroads and common roads by which inclined planes and hills may be ascended and heavy loads drawn up the same with more facility and economy than heretofore, and by which the evil effects of frost, ice, snows, and mud on the rail causing the wheels to slide are obviated."

— John Ruggles of Thomaston, Maine, invention patent, dated July 28, 1836.

Even after nearly two centuries of service, railroad technology continues to evolve. Like Ruggles, Argonne researchers and the rail industry are seeking ways to make railroad technology safer and more cost-effective — particularly in terms of a new generation of rail lubrication technology.

"We are assessing the environmental and tribological performance of a new railroad lubrication concept being proposed by Tranergy Corporation, an industrial partner," says Argonne's Mohumad Alzoubi. Tranergy, working with Texaco, has invented a computerized lubrication system — called SENTRAEN 2000™ — that applies top-of-rail (TOR) lubricant on both rails after the last axle of the last locomotive at the front of the train passes by. The problem has been that the railroad industry has yet to find a really effective rail lubrication technology. This one holds a lot of promise.

Explains Alzoubi, "A computerized system onboard the train precisely controls the amount of lubricant applied to the rails. The lubricant additives are formulated and applied in such a way that they function as a lubricant for a limited period. After the train passes over the lubricated sections, the lubricant degrades and no longer functions."

"We are investigating to confirm that the top-of-rail lubricant is environmentally cleaner than the moly [flange grease lubricant] and graphite grease being used today," says Alzoubi, adding that "the lubricant easily degrades, does not build up on the rails or wheels, and does not increase full-service braking distance." Other benefits are numerous: the technology could save the industry energy, increase productivity (fewer locomotives can be used to pull the same number of cars), cut track maintenance costs (less wear on wheels and tracks), and help prevent derailments. According to the American Association of Railroads, the system could save the railroad industry up to \$2 billion annually in energy and wheel/rail maintenance costs.

Alzoubi and his colleagues are collecting and qualitatively identifying any volatile and semivolatile degradation compounds produced by using TOR lubricant. "We are also determining

whether or not the compounds are environmentally safe, biodegradable, and nontoxic," he says. In addition to that work, he is investigating the effects of axle load, angle of attack, and quantity of lubricant on lateral friction forces, as well as the lubricant consumption time.

Alzoubi's research found that introducing TOR lubricant results in an almost 60% reduction in lateral friction force, which offers great potential for energy savings and wear reduction. "In terms of additional work," says Alzoubi, "we need to investigate how the lubricant performs in extreme cold (from 30°F to -50°F) and extreme heat (from 100°F to 150°F)." In addition, Alzoubi and his colleagues plan to characterize wear debris, run tests with laser-glazed wheels, and further analyze the degradation of the TOR lubricant under real-world conditions.

Research partners include the U.S. Department of Energy, Texaco Corporation, and Tranergy Corporation.

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Argonne is evaluating a computerized lubrication system developed by Tranergy Corporation that applies lubricant to both rails as the train passes by. Photos show the nozzle and tank components of the system.



LOOKING DOWN THE ROAD

It's been a busy summer here at the Laboratory. We've been involved in some exciting events and received a number of impressive awards (see FasTrax below). We've undertaken some new research projects that you'll read about in the next issue. Also, two of the big DOE Office of Transportation Technologies-sponsored student competitions took place in May and June. The final year of the Ethanol Vehicle Challenge was held in Ontario, Canada, and the first year of the FutureTruck competition was held at GM's Desert Proving Grounds in Arizona. Once again, the results of the competitions garnered national attention and impressed their sponsors and the general public. To find out more about the students' achievements during the competitions, please visit our web site (<http://www.transportation.anl.gov>) and check out "What's New in Student Competitions."

One of the new developments at the Laboratory this summer: related research projects involving the close-up study of diesel spray patterns and soot formation (described on pages 2 and 3.) Argonne's Advanced Photon Source makes it possible for us to examine these phenomena at closer range than we ever have before. The knowledge gained could lead to higher-performance, lower-emission injectors for modern automotive engines, as well as more efficient operation.

Another diagnostic technology developed by the technical staff here at Argonne, GCtool, is a computer software package that lets automotive designers try out different system configurations, without the expense and delays of building numerous prototypes (page 4).

The article on page 5 describes how scientists in the Energy Systems Division discovered that, although it is energy-intensive to produce from scratch, aluminum may yield some very attractive performance and environmental advantages over conventional steel.

Argonne staff are also working with the rail industry on finding ways to make railroad technology safer and more cost-effective (page 6).

We hope you've had a productive and fun summer too.



Please call or write to us and let us know what you're up to. We've added some new information to the back page of the newsletter to help remind you about how we can put Argonne's many resources to work for you.

Larry R. Johnson
Director
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FASTRAX

Bassam Jody and **Edward Daniels** of the Energy Systems Division and **Joseph Libera** (formerly of Argonne) received one of Argonne's three R&D 100 awards — which recognize the 100 most technologically significant new products of the last year — for their discovery of an effective process to recover flexible polyurethane foam from automobile shredder residue. The recipients will receive their awards at a banquet at Chicago's Museum of Science and Industry in September.

A froth flotation process to recover usable plastics from mixed plastics waste — developed by **Bassam Jody**, **Joseph Pomykala**, and **Edward Daniels** of the Energy Systems Division and **Bayram Arman** and **Dimitrios Karvelas** (formerly of Argonne) — was named a Finalist in the 2000 Discover Magazine Awards, presented annually to the best technologies developed by U.S. corporate, academic, and government research centers. The winners were honored at a ceremony at Disney World in Orlando, Florida, in June.

In May, **Raj Sekar** of the Energy Systems Division and **Ramesh Poola** (formerly of Argonne) received U.S. Patent No.

6,055,808, entitled "Method and Apparatus for Reducing Particulates and NO_x Emissions from Diesel Engines Utilizing Oxygen Enriched Combustion Air." The breakthrough technology, featured in *TransForum* Volume 2, No. 1, controls particulate and NO_x emissions in diesel engines.

Jules Roubort, of Argonne's Energy Technology Division, was invited to speak at the International Conference on "Mass and Charge Transport in Inorganic Materials: Fundamentals to Devices," held in Venice, Italy, on May 28–June 2, 2000. His lecture, "Creep in Electronic Ceramics," described Argonne's work to characterize minority defects that affect the conductivity of electrodes for fuel cells. The conference was attended by about 225 scientists from 20 countries.

Marianne Mintz, of Argonne's Energy Systems Division, has been named chair of the Transportation Energy Committee of the Transportation Research Board, which promotes theoretical and applied research on the energy and greenhouse gas emissions of transportation vehicles and fuels.



PUTTING ARGONNE'S RESOURCES TO WORK FOR YOU

Industrial technology development is an important way for the national laboratories to transfer the benefits of publicly funded research to industry to help strengthen the nation's technology base. The stories highlighted in this issue of *TransForum* represent some of the ways Argonne works with the transportation industry to improve processes, create products and markets, and lead the way to cost-effective transportation solutions, which in turn lead to a healthier economic future.

By working with Argonne through various types of cost-sharing arrangements, companies can jump-start their efforts to develop the next generation of transportation technologies without shouldering the often-prohibitive cost of initial R&D alone. Argonne has participated in dozens of these partnerships and has even been involved in helping to launch startup companies based on the products and technologies developed here.

If working with world-class scientists and engineers, having access to state-of-the-art user facilities and resources, and leveraging your company's own capabilities sound like good business opportunities to you, please contact our Office of Technology Transfer and see how we can put our resources to work for you.

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